An inverse scattering problem for the time-dependent Maxwell equations : nonlinear optimization and model-order reduction

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An Inverse Scattering Problem for the Time-Dependent Maxwell Equations: Nonlinear Optimization and Model-Order Reduction

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SUMMARY

In this paper an inverse scattering problem for the time-dependent Maxwell curl equations is considered. This problem is formulated as an optimal control problem governed by partial differential equations. First-order necessary optimality conditions are discussed. For the numerical solution a gradient-based algorithm is applied and successfully tested for some numerical examples. Finally, model-order reduction based on proper orthogonal decomposition is utilized to derive a reduced-order model for the time-dependent Maxwell curl equations. Its applicability is tested with respect to different input frequencies. Copyright © 2010 John Wiley & Sons, Ltd.

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KEY WORDS: Time-dependent Maxwell equations; inverse scattering; optimal control; nonlinear optimization; model reduction; proper orthogonal decomposition.

1. INTRODUCTION

Inverse scattering problems [2, 18, 19, 30, 33] are very important in noninvasive imaging. In fact, because electromagnetic (EM) waves can penetrate in various media, where objects may be placed, the solution of inverse scattering problems allows to determine the presence and the properties of these objects hidden in the medium. Hence, one should deal with Maxwell's equations. They can be considered either in frequency or in time domain. In this paper the time domain version is used. In fact, data in time domain are richer in information because of the large spectrum of possible frequency of the incident field. We focus on an unbounded domain, which arises in many applications, e.g., in mine detection [7]. Because of that, in the problem formulation we need to use an infinit radiation condition.

Optimal control problems for partial differential equations are often hard to tackle numerically so that the need for developing novel techniques emerges. One such technique is given by reduced-order methods. For a general overview we refer the reader to [1]. Recently the application of reduced-order models to optimal control problems has received an increasing amount of attention; see, e.g., [14, 25]. The reduced-order approach is based on projecting the dynamical system onto subspaces consisting of basis elements that contain characteristics of the expected solution. This is in contrast to, e.g., finite element techniques, where the elements of the subspaces are uncorrelated to the physical properties of the system that they approximate. In this work we concentrate on the method of proper orthogonal decomposition (POD) [15, 35] as one of the reduced-order approaches. Since the solution of Maxwell equations – especially in three dimensions – has a significant computational cost, we consider a POD Galerkin scheme for the FDTD scheme. The POD method is used here to reduce the EM fields. For other model order reduction technique in the EM context,

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Figure 1. A cross section of scenario for an inverse scattering problem in the domain Ω and scatterer domain $D \subsetneq \Omega$. The antennas with the circles are the transmitting antennas in the incidence position, while the antennas without circles are the receiving ones.

refer to [5, 6, 10, 12]. In [8] POD is applied for a finite difference discretization using a staggered grid. For an error estimate we refer to [31]. The authors consider parabolic equations and use a finite difference scheme as a high-dimensional discretization method. An error estimate is derived for the error between the solution to a parabolic equation and the associated POD Galerkin solution.

The paper is organized in the following manner: In Section 2 we formulate the inverse scattering problem as a nonlinear optimal control problem and present first-order necessary optimality conditions. The discretization of the optimality system is introduced in Section 3, where also numerical examples are shown. Section 4 is devoted on the proper orthogonal decomposition technique. Finally, we draw some conclusions in the last section.

2. EM INVERSE SCATTERING PROBLEM IN OPTIMIZATION FRAMEWORK

In this section, we formulate a time-domain electromagnetic (EM) inverse scattering problem in the framework of optimization with partial differential equations (PDEs) as constraints; [13, 34]. Our objective is to minimize a functional of EM field data misfit including a regularization functional for the EM properties that are sought. To characterize the solution of the resulting optimization problem, we derive the corresponding first-order optimality system.

2.1. Problem formulation

Consider the scenario illustrated in Figure 1. This scenario consists of an unbounded domain $\Omega \subset \mathbb{R}^3$. The boundary of Ω – if it exists – is denoted by Γ . Moreover, let $T > 0$ stand for the terminal time and $Q = (0, T) \times \Omega$. Let $D \subsetneq \Omega$ denote the *scatterer domain* and $Q_D = (0, T) \times D$. We suppose that $\Omega \setminus D$ has known EM properties, e.g., they can be the free space EM properties with electric permittivity $\varepsilon_0 > 0$, the magnetic permeability $\mu_0 > 0$ and conductivity $\sigma_0 = 0$. In the scatterer domain D we assume that the EM properties ε , μ , and σ depend on the spatial variable $\mathbf{x} \in D$ and that they are different from those of the background medium. Moreover, we consider multiple antennas and receivers surrounding the scatterer domain D . The *inverse scattering problem* consists in the problem of reconstructing the EM properties $\mathbf{p} = (\varepsilon, \mu, \sigma)$ in the scatterer domain without accessing in it, knowing the EM field only in some points of the domain $\Omega \setminus D$. Throughout the paper we always assume that the scatterers have non-dispersive and isotropic EM properties (for detailed definitions, see [11]).

The goal is to estimate the EM properties in the scatterer domain D by utilizing the time-dependent Maxwell curl equations as a mathematical model to predict the electrical and magnetic field $\mathbf{E}$, $\mathbf{H} : Q \rightarrow \mathbb{R}^3$ at k_m specified measurement points $\mathbf{x}_k^m \in \Omega \setminus D$, $1 \leq k \leq k_m$. We suppose that measurement data is available at the points $\mathbf{x}_k^m$. Since the EM properties $\mathbf{p} = (\varepsilon, \mu, \sigma)$ enter the Maxwell equations, we can identify these properties in D in such a way that the corresponding fields $\mathbf{E} = \mathbf{E}(\mathbf{p})$ and $\mathbf{H} = \mathbf{H}(\mathbf{p})$ are as close as possible to given data at the measurement points. In particular, we excite the Maxwell curl equations by n_i different sources in order to get

n_i field variables $(\mathbf{E}_n, \mathbf{H}_n)$, $1 \leq n \leq n_i$. We start with one incident wave in a certain position $\mathbf{x}_1^i \in \Omega \setminus D$. Then, we compute the associated EM fields $(\mathbf{E}_1, \mathbf{H}_1)$ in the k_m measurement points $\mathbf{x}_i^m$, $1 \leq k \leq k_m$ over the time interval $[0, T]$. Then, we repeat the same procedure for the other $n_i - 1$ incidence points.

We introduce the parameter space

$$\mathcal{P} = \mathbf{H}^1(D) \cap \mathbf{L}^\infty(D),$$

where $\mathbf{H}^1(D) = H^1(D) \times H^1(D) \times H^1(D)$ and $\mathbf{L}^\infty(D) = L^\infty(D) \times L^\infty(D) \times L^\infty(D)$. The set of admissible parameters by

$$\mathcal{P}_{\text{ad}} = \{(\varepsilon, \mu, \sigma) \in \mathcal{P} \mid \varepsilon_a \leq \varepsilon \leq \varepsilon_b, \mu_a \leq \mu \leq \mu_b, \sigma_a \leq \sigma \leq \sigma_b \text{ almost everywhere in } D\}$$

with positive lower and upper bounds $\varepsilon_a, \mu_a, \sigma_a, \varepsilon_b, \mu_b, \sigma_b \in L^\infty(D)$ satisfying $\varepsilon_a \leq \varepsilon_b, \mu_a \leq \mu_b, \sigma_a \leq \sigma_b$ in D almost everywhere. Then, for any parameter vector $\mathbf{p} \in \mathcal{P}_{\text{ad}}$ and for the n th incident wave ($1 \leq n \leq n_i$) the EM fields $(\mathbf{E}_n, \mathbf{H}_n)$ satisfy the Maxwell curl equations (see, e.g., [11, 28])

$$\begin{aligned} \nabla \times \mathbf{E}_n + \mu_0 \frac{\partial \mathbf{H}_n}{\partial t} &= 0 & \text{in } Q \setminus Q_D, \\ \nabla \times \mathbf{E}_n + \mu \frac{\partial \mathbf{H}_n}{\partial t} &= 0 & \text{in } Q_D, \\ \nabla \times \mathbf{H}_n - \varepsilon_0 \frac{\partial \mathbf{E}_n}{\partial t} - \mathbf{J}_n &= 0 & \text{in } Q \setminus Q_D, \\ \nabla \times \mathbf{H}_n - \varepsilon \frac{\partial \mathbf{E}_n}{\partial t} - \sigma \mathbf{E}_n &= 0 & \text{in } Q_D. \end{aligned} \quad (1a)$$

Together with (1a) we pose the initial conditions

$$\mathbf{E}_n(0, \cdot) = 0, \quad \mathbf{H}_n(0, \cdot) = 0 \quad \text{in } \Omega \quad (1b)$$

and the Sommerfeld radiation condition at infinity

$$\lim_{r \rightarrow \infty} r \left(\nabla \times \begin{pmatrix} \mathbf{E}_n \\ \mathbf{H}_n \end{pmatrix} + \frac{1}{c_0} \mathbf{n}_r \times \frac{\partial}{\partial t} \begin{pmatrix} \mathbf{E}_n \\ \mathbf{H}_n \end{pmatrix} \right) = 0 \quad \text{in } \Omega_r = \{\mathbf{x} \in \mathbb{R}^3 \mid |\mathbf{x}|_2 < r\}, \quad (1c)$$

where $k_0 = \omega \sqrt{\mu_0 \varepsilon_0} = 2\pi f \sqrt{\mu_0 \varepsilon_0}$ and $\mathbf{n}_r$ is the outward normal vector to $\partial\Omega_r$, the surface boundary of Ω_r . In (1c) we use that $D \subsetneq \Omega_r$ for sufficiently large radius r . Finally, we define the field excitation. We consider a hard source [32], i.e., we assign a time dependent excitation function to a field component while the density current $\mathbf{J}_n$ is zero:

$$\mathbf{H}_n(t, \mathbf{x}_n^i) = \mathbf{f}_n(t) \quad \text{in } (0, T). \quad (1d)$$

Remark 2.1

Let us mention that (1d) can be replaced by $\mathbf{E}_n(t, \mathbf{x}_n^i) = \tilde{\mathbf{f}}_n(t)$ in $(0, T)$. A third possibility is to apply different current densities $\mathbf{J}_n$ in (1a) for $n = 1, \dots, n_i$. $\diamond$

Assumption 1 (Existence and uniqueness for the Maxwell curl equations)

For any incident point $\mathbf{x}_n^i \in \Omega \setminus D$, $1 \leq n \leq n_i$, and for any $\mathbf{p} \in \mathcal{P}_{\text{ad}}$ there exist unique fields $\mathbf{E}_n$ and $\mathbf{H}_n$ satisfying

$$\mathbf{E}_n, \mathbf{H}_n \in C([0, T]; \mathbf{H}^1(\Omega) \cap C(\overline{\Omega})) \cap H^1(0, T; C(\overline{\Omega})) =: \mathcal{Y}_i$$

for $n = 1, \dots, n_i$, where $C(\overline{\Omega}) = C(\overline{\Omega}) \times C(\overline{\Omega}) \times C(\overline{\Omega})$.

Remark 2.2 1) The space $\mathcal{Y}_i$ is a Banach space endowed with the norm

$$\|\mathbf{G}\|_{\mathcal{Y}_i} = \max_{t \in [0, T]} \left(\|\mathbf{G}(t)\|_{\mathbf{H}^1(\Omega)} + \|\mathbf{G}(t)\|_{C(\overline{\Omega})} \right) + \left(\int_0^1 \|\mathbf{G}(t)\|_{C(\overline{\Omega})}^2 + \|\dot{\mathbf{G}}(t)\|_{C(\overline{\Omega})}^2 dt \right)^{1/2}$$

for $G \in \mathcal{Y}_i$. We define the Banach spaces

$$\mathcal{Y} = \underbrace{\mathcal{Y}_i \times \dots \times \mathcal{Y}_i}_{2n_i\text{-times}}, \quad \mathcal{X} = \mathcal{Y} \times \mathcal{P}$$

endowed with their natural product topology. Moreover let $\mathcal{X}_{\text{ad}} = \mathcal{Y} \times \mathcal{P}_{\text{ad}} \subset \mathcal{X}$.

- 2) For bounded domains, perfectly conducting boundary conditions and suitable smooth data it is shown in [20] that the Maxwell curl equations admits a unique solution.
- 3) If Assumption 1 holds true, we can define the solution operator $\mathcal{S} : \mathcal{P}_{\text{ad}} \rightarrow \mathcal{Y}$, where

$$(\mathbf{E}, \mathbf{H}) = \left((\mathbf{E}_n)_{n=1}^{n_i}, (\mathbf{H}_n)_{n=1}^{n_i} \right) = \mathcal{S}(\mathbf{p}), \quad \mathbf{p} = (\varepsilon, \mu, \sigma) \in \mathcal{P}_{\text{ad}},$$

denotes the solution pairs to (1) for the n_i incident waves. Due to the three bilinear terms $\mu \frac{\partial \mathbf{H}_n}{\partial t}$, $\varepsilon \frac{\partial \mathbf{E}_n}{\partial t}$ and $\sigma \mathbf{E}_n$ the operator $\mathcal{S}$ is nonlinear. $\diamond$

To write the inverse scattering problem as an optimization problem, we define a cost functional that penalizes the discrepancies between the measured data and the calculated fields. We aim at minimizing the misfit by varying the unknown EM properties in D which define the optimization variables. Because of the ill-posedness of the inverse problem, we include a regularization term, $R(\mathbf{p})$. Thus we introduce the cost functional $\mathcal{J} : \mathcal{X} \rightarrow \mathbb{R}$ by

$$\mathcal{J}(\mathbf{X}) = \frac{1}{2} \sum_{n=1}^{n_i} \sum_{k=1}^{k_m} \int_0^T (|\mathbf{E}_{nk}(t) - \mathbf{E}_{nk}^m(t)|_2^2 + \eta_0^2 |\mathbf{H}_{nk}(t) - \mathbf{H}_{nk}^m(t)|_2^2) dt + R(\mathbf{p}), \quad (2)$$

where $\mathbf{X} = (\mathbf{E}, \mathbf{H}, \mathbf{p}) \in \mathcal{X}$, $\mathbf{E} = (\mathbf{E}_1, \dots, \mathbf{E}_{n_i})$, $\mathbf{H} = (\mathbf{H}_1, \dots, \mathbf{H}_{n_i})$, $|\cdot|_2$ denotes the Euclidean norm, $\eta_0 > 0$ is the characteristic impedance of free space, $\mathbf{E}_{nk} = \mathbf{E}_n(\cdot, \mathbf{x}_k^m)$ and $\mathbf{H}_{nk}(\cdot, \mathbf{x}_k^m)$ are the computed evaluated in the k th measurement point for the n th incident wave fields, whereas $\mathbf{E}_{nk}^m$ and $\mathbf{H}_{nk}^m$ are the associated measurement data. We consider the following regularization term

$$\begin{aligned} R(\mathbf{p}) = & \frac{\beta}{2} \int_D |\nabla \varepsilon(\mathbf{x})|^2 + |\nabla \sigma(\mathbf{x})|^2 + |\nabla \mu(\mathbf{x})|^2 d\mathbf{x} \\ & + \frac{\gamma}{2} \int_D |\varepsilon(\mathbf{x}) - \bar{\varepsilon}(\mathbf{x})|^2 + |\sigma(\mathbf{x}) - \bar{\sigma}(\mathbf{x})|^2 + |\mu(\mathbf{x}) - \bar{\mu}(\mathbf{x})|^2 d\mathbf{x} \end{aligned} \quad (3)$$

for $\mathbf{p} = (\varepsilon, \mu, \sigma) \in \mathcal{P}$. In this regularization functional we distinguish two different terms. The first term represents a first-order Tikhonov regularization scheme. Minimizing the functional $\mathcal{J}$ with this type of regularization means that we search the model parameters $\mathbf{p}$ in a smooth space with spatially slow varying functions. A result of this choice is that we obtain the edges of the reconstructed objects smeared out by diffusion. The other regularization term represents a zero-order Tikhonov regularization and corresponds to the requirement that ε is as close as possible to a given nominal $\bar{\varepsilon}$, and similarly σ is as close as possible to $\bar{\sigma}$, and μ is as close as possible to $\bar{\mu}$. This regularization term can be used even if we do not have a priori information with known $\bar{\mathbf{p}} = (\bar{\varepsilon}, \bar{\mu}, \bar{\sigma})$. In this case we choose these values to be zero and the resulting regularization term penalizes large parameters values.

Now, the inverse scattering problem is expressed as the infinite-dimensional, nonlinear optimization problem

$$\min \mathcal{J}(\mathbf{X}) \quad \text{subject to (s.t.)} \quad \text{the pair } \mathbf{X} = (\mathbf{E}, \mathbf{H}, \mathbf{p}) \in \mathcal{X}_{\text{ad}} \text{ and } (\mathbf{E}, \mathbf{H}) = \mathcal{S}(\mathbf{p}). \quad (\mathbf{P})$$

If Assumption 1 is satisfied, we can introduce the *reduced cost functional* $\hat{\mathcal{J}} : \mathcal{P}_{\text{ad}} \rightarrow \mathbb{R}$ by

$$\hat{\mathcal{J}}(\mathbf{p}) = \mathcal{J}(\mathcal{S}(\mathbf{p}), \mathbf{p}), \quad \mathbf{p} \in \mathcal{P}_{\text{ad}}.$$

Then, (P) can be equivalently expressed as the *reduced problem*

$$\min \hat{\mathcal{J}}(\mathbf{p}) \quad \text{s.t.} \quad \mathbf{p} \in \mathcal{P}_{\text{ad}}. \quad (\hat{\mathbf{P}})$$

Assumption 2 (Existence of optimal solutions)

Problem **(P)** admits at least one local optimal solution $\mathbf{X}^* = (\mathbf{E}^*, \mathbf{H}^*, \mathbf{p}^*) \in \mathcal{X}_{\text{ad}}$. Moreover, $\mathbf{p}^* = (\varepsilon^*, \mu^*, \sigma^*)$ is an interior point of $\mathcal{P}_{\text{ad}}$, i.e., $\varepsilon_a < \varepsilon^* < \varepsilon_b$, $\mu_a < \mu^* < \mu_b$ and $\sigma_a < \sigma^* < \sigma_b$ in D almost everywhere.

Remark 2.3 1) Let Assumption 2 hold. Then, $\mathbf{p}^*$ solves $(\hat{\mathbf{P}})$.

2) Suppose that Assumption 2 is satisfied. Then, $\mathbf{p}^*$ is a local solution to

$$\min \hat{\mathcal{J}}(\mathbf{p}) \quad \text{s.t.} \quad \mathbf{p} \in \mathcal{P}. \quad (\hat{\mathbf{P}}_{\text{eq}})$$

In this case we can neglect the inequality constraints for the parameter $\mathbf{p}$. Together with the associated state $(\mathbf{E}^*, \mathbf{H}^*) = \mathcal{S}(\mathbf{p}^*)$ the triple $\mathbf{X}^* = (\mathbf{E}^*, \mathbf{H}^*, \mathbf{p}^*)$ is a local solution $\mathbf{p}^*$ to the equality constrained problem

$$\min \mathcal{J}(\mathbf{X}) \quad \text{s.t.} \quad \text{the pair } \mathbf{X} = (\mathbf{E}, \mathbf{H}, \mathbf{p}) \in \mathcal{X} \text{ and } (\mathbf{E}, \mathbf{H}) = \mathcal{S}(\mathbf{p}). \quad (\mathbf{P}_{\text{eq}})$$

In the numerical experiments carried out in Section 3.2 we apply a gradient-type algorithm to $(\hat{\mathbf{P}}_{\text{eq}})$ respectively $(\mathbf{P}_{\text{eq}})$. $\diamond$

2.2. First-order necessary optimality conditions

Problem $(\hat{\mathbf{P}}_{\text{eq}})$ is an infinite-dimensional, constrained optimization problem. Thus, we apply techniques from PDE-optimization [13, 16, 34]. For this purpose we introduce the following Hilbert spaces

$$\mathcal{Z}_i = L^2(0, T; \mathbf{H}^1(\Omega)) \cap H^1(0, T; \mathbf{L}^2(\Omega)), \quad \mathcal{Z} = \underbrace{\mathcal{Z}_1 \times \dots \times \mathcal{Z}_{n_i}}_{2n_i\text{-times}}$$

with the natural product topology and define the Lagrange functional $\mathcal{L} : \mathcal{X} \times \mathcal{Z} \rightarrow \mathbb{R}$ by

$$\begin{aligned} \mathcal{L}(\mathbf{X}, \Lambda) = & \mathcal{J}(\mathbf{X}) + \sum_{n=1}^{n_i} \int_0^T \int_{\Omega} \left(\lambda_n^E \cdot \left(\nabla \times \mathbf{H}_n - \varepsilon \frac{\partial \mathbf{E}_n}{\partial t} - \sigma \mathbf{E}_n - \mathbf{J}_n \right) \right) d\mathbf{x} dt \\ & + \sum_{n=1}^{n_i} \int_0^T \int_{\Omega} \left(\lambda_n^H \cdot \left(\nabla \times \mathbf{E}_n + \mu \frac{\partial \mathbf{H}_n}{\partial t} \right) \right) d\mathbf{x} dt, \end{aligned} \quad (4)$$

where $\mathbf{X} = (\mathbf{E}, \mathbf{H}, \mathbf{p}) \in \mathcal{X}$, $\Lambda = (\lambda^E, \lambda^H) \in \mathcal{Z}$ with $\lambda^E = (\lambda_1^E, \dots, \lambda_{n_i}^E)$, $\lambda^H = (\lambda_1^H, \dots, \lambda_{n_i}^H)$ and $\lambda_i^E, \lambda_i^H \in \mathcal{Z}_i$ for $1 \leq i \leq n_i$.

To solve the constrained minimization problem numerically, we want to make use of the first-order optimality conditions. If one can ensure the existence of Lagrange multipliers [22], an optimal solution $\mathbf{X}^*$ to $(\mathbf{P}_{\text{eq}})$ can be characterized by a stationary point of the Lagrange functional. Let Assumptions 1 and 2 hold. By $\mathbf{X}^* = (\mathbf{E}^*, \mathbf{H}^*, \mathbf{p}^*) \in \mathcal{X}_{\text{ad}}$ we denote a local optimal solution to $(\mathbf{P}_{\text{eq}})$. Moreover, let $\mathbf{Y}^* = (\mathbf{E}^*, \mathbf{H}^*) = \mathcal{S}(\mathbf{p}^*) \in \mathcal{Y}$.

Assumption 3 (First-order necessary optimality conditions)

The Lagrangian $\mathcal{L}$ is continuously Fréchet-differentiable. Moreover, exists an associated pair of Lagrange multipliers $\Lambda^* = (\lambda^{E,*}, \lambda^{H,*}) \in \mathcal{Z}$ satisfying the following first-order necessary optimality conditions:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{Y}}(\mathbf{X}^*, \Lambda^*) \mathbf{Y} = 0 \quad \text{for all } \mathbf{Y} = (\mathbf{E}, \mathbf{H}) \in \mathcal{Y}, \quad (5a)$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{p}}(\mathbf{X}^*, \Lambda^*) \mathbf{p} = 0 \quad \text{for all } \mathbf{p} \in \mathcal{P}, \quad (5b)$$

where $\frac{\partial \mathcal{L}}{\partial \mathbf{Y}}, \frac{\partial \mathcal{L}}{\partial \mathbf{p}}$ denote the Fréchet derivatives of the Lagrangian $\mathcal{L}$ with respect to $\mathbf{Y}$, and $\mathbf{p}$, respectively.

Remark 2.4

The existence of Lagrange multipliers can be ensured by constraint qualification conditions; see [16, 22, 34], for instance. Due to (1c) the proof is not evident in our case. $\diamond$

With Assumption 3 holding, we proceed formally by computing the directional derivatives of the Lagrange functional. For the details we refer the reader to the thesis [21].

From (5a) we infer that the pair $\Lambda = (\lambda^{E,*}, \lambda^{H,*}) \in \mathcal{Z}$ satisfies the following adjoint system

$$\begin{aligned}
\nabla \times \lambda_n^{E,*} - \mu_0 \frac{\partial \lambda_n^{H,*}}{\partial t} &= 0 & \text{in } Q \setminus Q_D, \\
\nabla \times \lambda_n^{E,*} - \mu \frac{\partial \lambda_n^{H,*}}{\partial t} + \eta_0^2 \sum_{k=1}^{k_m} (\mathbf{H}_n^* - \mathbf{H}_n^m) \delta_{\mathbf{x}_k^m} &= 0 & \text{in } Q_D, \\
\nabla \times \lambda_n^{H,*} + \varepsilon_0 \frac{\partial \lambda_n^{E,*}}{\partial t} &= 0 & \text{in } Q \setminus Q_D, \\
\nabla \times \lambda_n^{H,*} + \varepsilon \frac{\partial \lambda_n^{E,*}}{\partial t} - \sigma \lambda_n^{E,*} + \sum_{k=1}^{k_m} (\mathbf{E}_n^* - \mathbf{E}_n^m) \delta_{\mathbf{x}_k^m} &= 0 & \text{in } Q_D, \\
\lambda_n^{E,*}(T, \cdot) = 0, \quad \lambda_n^{H,*}(T, \cdot) &= 0 & \text{in } \Omega, \\
\lim_{r \rightarrow \infty} r \left(\nabla \times \begin{pmatrix} \lambda_n^{E,*} \\ \lambda_n^{H,*} \end{pmatrix} + \frac{1}{c_0} \mathbf{n}_r \times \frac{\partial}{\partial t} \begin{pmatrix} \lambda_n^{E,*} \\ \lambda_n^{H,*} \end{pmatrix} \right) &= 0 & \text{in } \Omega_r = \{\mathbf{x} \in \mathbb{R}^3 \mid |\mathbf{x}|_2 < r\}
\end{aligned} \tag{6}$$

for every incidence $n \in \{1, \dots, n_i\}$. In (6) we denote by $\delta_{\mathbf{x}_k^m} : C(\overline{D}) \rightarrow \mathbb{R}$ the Dirac delta mapping satisfying $\delta_{\mathbf{x}_k^m}(\mathbf{x}) = 1$ if $\mathbf{x} = \mathbf{x}_k^m$ holds. Otherwise, we have $\delta_{\mathbf{x}_k^m}(\mathbf{x}) = 0$.

Let us have a closer look to system (6). Lagrange multipliers satisfy Maxwell-like equations, in which the signs of the time derivatives are opposite with respect to the standard curl equations. Moreover, we see that they satisfy terminal conditions and particular boundary conditions, in which there is a change in the time derivative. It can be shown that Lagrange multipliers $\lambda_n^{E,*}$ and $\lambda_n^{H,*}$ are special kind of EM fields [21, 29]. In particular, they run backward in time, i.e., from $t = T$ to $t = 0$. We remark also the fact that these particular fields are excited by the discrepancies between the measurements and the predictions of the model in the k_m measurement points. If the model could exactly fit the scenario, i.e. the predictions of the model fit the measurements, the adjoint fields would have zero sources.

From (5b) we deduce the following equations in the dual space $H^1(D)'$ of $H^1(D)$

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \varepsilon}(\mathbf{X}^*, \Lambda^*) &= -\beta \Delta \varepsilon^* + \gamma(\varepsilon^* - \bar{\varepsilon}) - \sum_{n=1}^{n_i} \int_0^T \frac{\partial \mathbf{E}_n^*}{\partial t} \cdot \lambda_n^{E,*} dt = 0, \\
\frac{\partial \mathcal{L}}{\partial \mu}(\mathbf{X}^*, \Lambda^*) &= -\beta \Delta \mu^* + \gamma(\mu^* - \bar{\mu}) + \sum_{n=1}^{n_i} \int_0^T \frac{\partial \mathbf{H}_n^*}{\partial t} \cdot \lambda_n^{H,*} dt = 0, \\
\frac{\partial \mathcal{L}}{\partial \sigma}(\mathbf{X}^*, \Lambda^*) &= -\beta \Delta \sigma^* + \gamma(\sigma^* - \bar{\sigma}) - \sum_{n=1}^{n_i} \int_0^T \mathbf{E}_n^* \cdot \lambda_n^{E,*} dt = 0.
\end{aligned}$$

It can be shown [13] that the gradient $\hat{\mathcal{J}}'(\mathbf{p})$ of the reduced cost functional $\hat{\mathcal{J}}$ at a given parameter $\mathbf{p} \in \mathbf{H}^1(D)$ is given by the following functional:

$$\begin{aligned}
\hat{\mathcal{J}}'(\mathbf{p}) &= \left(-\beta \Delta \varepsilon + \gamma(\varepsilon - \bar{\varepsilon}) - \sum_{n=1}^{n_i} \int_0^T \frac{\partial \mathbf{E}_n}{\partial t} \cdot \lambda_n^E dt, \right. \\
&\quad \left. -\beta \Delta \mu + \gamma(\mu - \bar{\mu}) + \sum_{n=1}^{n_i} \int_0^T \frac{\partial \mathbf{H}_n}{\partial t} \cdot \lambda_n^H dt, \right. \\
&\quad \left. -\beta \Delta \sigma + \gamma(\sigma - \bar{\sigma}) - \sum_{n=1}^{n_i} \int_0^T \mathbf{E}_n \cdot \lambda_n^E dt \right) : \mathbf{H}^1(D) \rightarrow \mathbb{R}^3,
\end{aligned} \tag{7}$$

where $(\mathbf{E}, \mathbf{H}) = \mathcal{S}(\mathbf{p})$ and $\Lambda \in \mathcal{Z}$ solve (6) for $1 \leq n \leq n_i$. Hence, we use these three equations in our gradient-based optimization method for updating the EM properties in the scatterer domain D .

Figure 2. Spatial staggered grid arrangement for the TE_z wave.

For the update we have to solve the state equation (1) for the given parameter $\mathbf{p}$ and we have to determine the solution $\mathbf{\Lambda}$ to the adjoint equations.

3. DISCRETIZATION OF THE OPTIMALITY SYSTEM

There are several techniques for discretizing Maxwell equations (consider [17] for having a detailed overview of the most used techniques). We considered the finite difference time domain (FDTD) algorithm. For details about the method, we refer the reader to [9, 32, 36]. For convergence results we refer the reader to [23], where the authors consider the Maxwell curl equations with simpler – compared to the Sommerfeld radiation condition (1c) – boundary conditions.

3.1. The FDTD scheme

The discussion in Section 2 is valid in the general case of a three dimensional domain. Now we restrict ourselves to the two dimensional case, i.e., we do not consider variation in the z -direction (see [11, 32]). In this context, one can have two different types of waves: *transverse electric* (TE_z) and *transverse magnetic* (TM_z). We focus on the TE_z case, which has the fields components E_x , E_y and H_z : $\mathbf{E}_n = (E_x, E_y, 0)^\top$ and $\mathbf{H}_n = (0, 0, H_z)^\top$. For every incident wave n , they are coupled accordingly to the following system

$$\begin{aligned} \frac{\partial E_x}{\partial t} &= \frac{1}{\varepsilon_0} \left(\frac{\partial H_z}{\partial y} - J_{sx} \right) & \text{in } Q \setminus Q_D, & \quad \frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon} \left(\frac{\partial H_z}{\partial y} - (J_{sx} + \sigma E_x) \right) & \text{in } Q_D, \\ \frac{\partial E_y}{\partial t} &= \frac{1}{\varepsilon_0} \left(-\frac{\partial H_z}{\partial x} - J_{sy} \right) & \text{in } Q \setminus Q_D, & \quad \frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon} \left(-\frac{\partial H_z}{\partial x} - (J_{sy} + \sigma E_y) \right) & \text{in } Q_D, \\ \frac{\partial H_z}{\partial t} &= \frac{1}{\mu_0} \left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right) & \text{in } Q \setminus Q_D, & \quad \frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right) & \text{in } Q_D, \end{aligned}$$

where we skipped the index n .

We consider the FDTD method for discretizing the TE_z system. The FDTD scheme is characterized by the fact that the field components are considered in a staggered grid in space and in time. In our case, the spatial arrangement of the fields component is like in Figure 2.

This implies that if we consider a space grid of dimension $M \times N$ for H_z , there will be $M \times (N + 1)$ points for E_x and $(M + 1) \times N$ for E_y . For simplicity, we consider the case of an uniform grid, so we have the step sizes Δx and Δy on x and y directions, respectively. Moreover, magnetic and electric fields are interleaved in time. Calling Δt the time step and N_t the number of time-steps, we evaluate E_x and E_y in the time instants $(m + 1/2)\Delta t$ and H_z in the time instants $m\Delta t$, with $m = 0, \dots, N_t$. It is worth noting that time step Δt and step sizes Δx and Δy are related by the Courant condition [9, 32]. Considering a square space grid, in which $h = \Delta x = \Delta y$, if one choose the time step Δt then Δ should be taken in order to fulfill $c\sqrt{2}\Delta t < h$, where c is the speed in the vacuum. On the space-time grid, we consider $E_x(i\Delta x, (j - 1/2)\Delta y; (m + 1/2)\Delta t) \approx E_{x,i,j-1/2}^{m+1/2}$, $E_y((i - 1/2)\Delta x, j\Delta y; (m + 1/2)\Delta t) \approx E_{y,i-1/2,j}^{m+1/2}$ and $H_z(i\Delta x, j\Delta y; m\Delta t) \approx H_{z,i,j}^{m+1}$.

Figure 3. Elementary cell for the TE_z case.

for $i = 1, \dots, M$ and $j = 1, \dots, N$, $m = 0, \dots, N_t$. Identifying the elementary cell by the couple of index (I, J) as in Figure 3, the discrete system is given by

$$\begin{aligned}
 E_{x,I,J}^{m+1/2} &= \frac{2\varepsilon_{x,I,J} - \Delta t \sigma_{x,I,J}}{2\varepsilon_{x,I,J} + \Delta t \sigma_{x,I,J}} E_{x,I,J}^{m-1/2} + \frac{2\Delta t}{2\varepsilon_{x,I,J} + \Delta t \sigma_{x,I,J}} \left(\frac{H_{z,I,J}^m - H_{z,I,J-1}^m}{\Delta x} - J_{sx,I,J}^m \right), \\
 &\quad I = 1, \dots, M, \quad J = 2, \dots, N \\
 E_{y,I,J}^{m+1/2} &= \frac{2\varepsilon_{y,I,J} - \Delta t \sigma_{y,I,J}}{2\varepsilon_{y,I,J} + \Delta t \sigma_{y,I,J}} E_{y,I,J}^{m-1/2} + \frac{2\Delta t}{2\varepsilon_{y,I,J} + \Delta t \sigma_{y,I,J}} \left(\frac{H_{z,I-1,J}^m - H_{z,I,J}^m}{\Delta x} - J_{sy,I,J}^m \right), \\
 &\quad I = 2, \dots, M, \quad J = 1, \dots, N, \\
 H_{z,I,J}^{m+1} &= H_{z,I,J}^m + \frac{\Delta t}{\mu_{I,J}} \left(\frac{E_{y,I,J}^{m+1/2} - E_{y,I+1,J}^{m+1/2}}{\Delta x} - \frac{E_{x,I,J+1}^{m+1/2} - E_{x,I,J}^{m+1/2}}{\Delta y} \right), \\
 &\quad I = 1, \dots, M, \quad J = 1, \dots, N \\
 &\quad m = 0, \dots, N_t.
 \end{aligned}$$

Clearly, these equations provide an update for the inner grid points. This means that we need other equations for updating the boundary values of E_x and E_y . Since we consider an unbounded domain, we update the fields in these points using some absorbing boundary condition (ABC) equations. A very popular ABC in the FDTD community is the perfectly matched layer (PML) [3]. In this approach, one surround the computational domain with a certain number of cells of an anisotropic, lossy medium, in which there are σ_x , σ_y , σ_x^* and σ_y^* , where the latter 2 are the magnetic conductivities. Because of the anisotropy, in the PML region one need to split the the H_z field component, i.e., one need to consider H_{zx} and H_{zy} . Since next we would like to consider a model reduction technique, we consider another ABC, in order to avoid the reduction of the split field components. We have used the second order Mur scheme [32], that follows from the Engquist-Majda one-way wave equations which are

$$\begin{aligned}
 \frac{\partial E_x}{\partial t} &= c \frac{\partial E_x}{\partial y} && \text{for the lower bound,} \\
 \frac{\partial E_x}{\partial t} &= -c \frac{\partial E_x}{\partial y} && \text{for the upper bound,} \\
 \frac{\partial E_y}{\partial t} &= c \frac{\partial E_y}{\partial x} && \text{for the left bound,} \\
 \frac{\partial E_y}{\partial t} &= -c \frac{\partial E_y}{\partial x} && \text{for the right bound,}
 \end{aligned}$$

where $c > 0$ is the speed of the light in the vacuum. Using central differences, we get the second-order Mur absorbing boundary conditions for the E_x component [24]

$$E_{x,I,1}^{m+1/2} = -E_{x,I,2}^{m-3/2} + \frac{c\Delta t - \Delta y}{c\Delta t + \Delta y} \left(E_{x,I,2}^{m+1/2} + E_{x,I,1}^{m-3/2} \right) + \frac{2\Delta y}{c\Delta t + \Delta y} \left(E_{x,I,1}^{m-1/2} + E_{x,I,2}^{m-1/2} \right) \\ + \frac{(c\Delta t)^2}{2\Delta y(c\Delta t + \Delta y)} \left(E_{x,I+1,1}^{m-1/2} - 2E_{x,I,1}^{m-1/2} + E_{x,I-1,1}^{m-1/2} + E_{x,I+1,2}^{m-1/2} - 2E_{x,I,2}^{m-1/2} + E_{x,I-1,2}^{m-1/2} \right)$$

for $I = 2, \dots, M-1$ and $m = 0, \dots, N_t$,

$$E_{x,I,N+1}^{m+1/2} = -E_{x,I,N}^{m-3/2} + \frac{c\Delta t - \Delta y}{c\Delta t + \Delta y} \left(E_{x,I,N}^{m+1/2} + E_{x,I,N+1}^{m-3/2} \right) + \frac{2\Delta y}{c\Delta t + \Delta y} \left(E_{x,I,N}^{m-1/2} + E_{x,I,N+1}^{m-1/2} \right) \\ + \frac{(c\Delta t)^2}{2\Delta y(c\Delta t + \Delta y)} \left(E_{x,I+1,N}^{m-1/2} - 2E_{x,I,N}^{m-1/2} + E_{x,I-1,N}^{m-1/2} \right) \\ + \frac{(c\Delta t)^2}{2\Delta y(c\Delta t + \Delta y)} \left(E_{x,I+1,N+1}^{m-1/2} - 2E_{x,I,N+1}^{m-1/2} + E_{x,I-1,N+1}^{m-1/2} \right)$$

for $i = 2, \dots, M-1$ and $m = 0, \dots, N_t$,

$$E_{x,1,1}^{m+1/2} = E_{x,1,2}^{m-1/2} + \frac{c\Delta t - \Delta y}{c\Delta t + \Delta y} \left(E_{x,1,2}^{m+1/2} - E_{x,1,1}^{m-1/2} \right), \\ E_{x,M,1}^{m+1/2} = E_{x,M,2}^{m-1/2} + \frac{c\Delta t - \Delta y}{c\Delta t + \Delta y} \left(E_{x,M,2}^{m+1/2} - E_{x,M,1}^{m-1/2} \right), \\ E_{x,1,N+1}^{m+1/2} = E_{x,1,N}^{m-1/2} + \frac{c\Delta t - \Delta y}{c\Delta t + \Delta y} \left(E_{x,1,N}^{m+1/2} - E_{x,1,N+1}^{m-1/2} \right), \\ E_{x,M,N+1}^{m+1/2} = E_{x,M,N}^{m-1/2} + \frac{c\Delta t - \Delta y}{c\Delta t + \Delta y} \left(E_{x,M,N}^{m+1/2} - E_{x,M,N+1}^{m-1/2} \right),$$

for $m = 0, \dots, N_t$.

Analogously, we get the equations for the field component E_y .

Hence, we have all the equations we need for updating the fields components in the computational grid: this means that we have a discrete scheme for solving the direct problem. We can combine the update equations in a compact matrix notation. For that purpose we define the vectors $\mathbf{E}_x^{m+1/2} \in \mathbb{R}^{M(N+1)}$, $\mathbf{E}_y^{m+1/2} \in \mathbb{R}^{N(M+1)}$, $\mathbf{H}_z^{m+1} \in \mathbb{R}^{NM}$ for $m = 0, \dots, N_t$

$$\mathbf{E}_x^{m+1/2} = \left(E_{x,1,1}^{m+1/2}, \dots, E_{x,M,1}^{m+1/2}, E_{x,1,2}^{m+1/2}, \dots, E_{x,M,2}^{m+1/2}, E_{x,1,N+1}^{m+1/2}, \dots, E_{x,M,N+1}^{m+1/2} \right)^\top, \\ \mathbf{E}_y^{m+1/2} = \left(E_{y,1,1}^{m+1/2}, \dots, E_{y,M+1,1}^{m+1/2}, E_{y,1,2}^{m+1/2}, \dots, E_{y,M+1,2}^{m+1/2}, E_{y,1,N}^{m+1/2}, \dots, E_{y,M+1,N}^{m+1/2} \right)^\top, \\ \mathbf{H}_z^{m+1} = \left(H_{z,1,1}^{m+1}, \dots, H_{z,M,1}^{m+1}, H_{z,1,2}^{m+1}, \dots, H_{z,M,2}^{m+1}, H_{z,1,N}^{m+1}, \dots, H_{z,M,N}^{m+1} \right)^\top.$$

Then, the new iterates $\mathbf{E}_x^{m+1/2}$, $\mathbf{E}_y^{m+1/2}$ and $\mathbf{H}_z^{m+1}$ are computed as follows: Solve the linear system

$$\begin{pmatrix} \mathbf{M}_x & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_y \end{pmatrix} \begin{pmatrix} \mathbf{E}_x^{m+1/2} \\ \mathbf{E}_y^{m+1/2} \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{E_x} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_{E_y} \end{pmatrix} \begin{pmatrix} \mathbf{E}_x^{m-1/2} \\ \mathbf{E}_y^{m-1/2} \end{pmatrix} + \begin{pmatrix} \mathbf{A}_y \mathbf{H}_z^m + \mathbf{J}_{sx}^m \\ \mathbf{A}_x \mathbf{H}_z^m + \mathbf{J}_{sy}^m \end{pmatrix} \quad (8a)$$

and set

$$\mathbf{H}_z^{m+1} = \mathbf{H}_z^m + \mathbf{B}_y \mathbf{E}_x^{m+1/2} - \mathbf{B}_x \mathbf{E}_y^{m+1/2}, \quad (8b)$$

where $\mathbf{M}_x$, $\mathbf{M}_y$, $\mathbf{A}_{E_x}$, $\mathbf{A}_{E_y}$, $\mathbf{A}_x$, $\mathbf{A}_y$, $\mathbf{B}_x$, $\mathbf{B}_y$ are matrices that contain the discretization coefficients.

Next we consider now the discretization of the adjoint problem. Recall that the adjoint fields λ_n^E and λ_n^H are ingoing waves, with terminal conditions instead of initial conditions, i.e., they backpropagate in time starting from a final condition. In principle, we need a discretization scheme that runs with a decreasing time variable, in order to take into account this characteristic. In practice

we can avoid this and using the same FDTD used for solving the direct problem, after performing the transformation $\tilde{t} = T - t$ and thus compute the modified Lagrange multipliers that are solution of the following system of equations

$$\begin{aligned} \nabla \times \tilde{\lambda}_n^E + \mu_0 \frac{\partial \tilde{\lambda}_n^H}{\partial t} &= 0 && \text{in } Q \setminus Q_D, \\ \nabla \times \tilde{\lambda}_n^E + \mu \frac{\partial \tilde{\lambda}_n^H}{\partial t} + \eta_0^2 \sum_{k=1}^{k_m} (\tilde{H}_n - \tilde{H}_n^m) \delta_{x_k^m} &= 0 && \text{in } Q_D \\ \nabla \times \tilde{\lambda}_n^H + \varepsilon_0 \frac{\partial \tilde{\lambda}_n^E}{\partial t} &= 0 && \text{in } Q \setminus Q_D, \\ \nabla \times \tilde{\lambda}_n^H + \varepsilon \frac{\partial \tilde{\lambda}_n^E}{\partial t} - \sigma \tilde{\lambda}_n^E + \sum_{k=1}^{k_m} (\tilde{E}_n - \tilde{E}_n^m) \delta_{x_k^m} &= 0 && \text{in } Q_D. \end{aligned}$$

In fact, with the change of the time coordinate, the procedure used to compute $\tilde{\lambda}_n^E$ and $\tilde{\lambda}_n^H$ goes forward in time. At the end of the FDTD run for the modified Lagrange fields, the adjoint fields λ_n^E and λ_n^H can be obtained reading the results from the final one to the first.

After solving forward and adjoint problem, we can approximate numerically the gradient components of the reduced cost functional $\hat{J}(p)$ described in equations (7). The time derivatives are calculated using central differences approximation in time. We computed the time integration of the product terms using the trapezoidal rule. The terms related to the first-order regularization require the computation of a Laplace operator Δ . This operator is approximated using the five-point stencil rule. Having the gradient components, we can use them in an iterative scheme which updates the EM properties.

We have considered a steepest descent method. Hence, in the minimization problem of the functional $\hat{J}$, one can find a descent direction d_i as $d_i = -\hat{J}'(p_i) \in \mathbf{H}^1(D)'$ for every iteration i of the optimization scheme. Then, the update of the optimization variables is performed by $p_{i+1} = p_i + s_i \tilde{d}_i$, where s_i is a step length and $\tilde{d}_i = (\tilde{d}_i^\varepsilon, \tilde{d}_i^\mu, \tilde{d}_i^\sigma) \in \mathbf{H}^1(D)$ is the weak solution to the Neumann boundary value problem

$$-\Delta \tilde{d}_i + \tilde{d}_i = d_i \text{ in } D, \quad \frac{\partial \tilde{d}_i}{\partial \mathbf{n}} = 0 \text{ on } \partial D.$$

We considered also the BFGS for finding at every step a new descent direction, but we did not observe remarkable improvements in the speed of the reconstruction algorithm.

The line search method gives us the step length s_i , i.e., it tells how much to move on the descent direction d_i . We considered a backtracking procedure that stopped once the Armijo condition was satisfied (see, e.g., [26]).

3.2. A numerical example

In this subsection we consider a numerical example. We focus on the reconstruction of a dielectric scatterer. The algorithm is valid for multiple scatterers and/or magnetic and conductive scatterers, too.

In our experiment, the computational domain is a square whose side-length is three times larger than that of the scatterer square domain D . We assume the side-length of D corresponding to a length of 20 cells. The number of time steps is set to $N_t = 200$ and the time-step size is $\Delta t = 10^{-6}$ seconds. The time domain is $(0, T)$ where $T = N_t \Delta t$ seconds. The spatial increment, h is equal in the x - and y -direction and it is set equal to $h = 2 c \Delta t = 5.99 \cdot 10^2$ meters, such that it satisfies the Courant limit [32]. The EM properties of the background are those one of the free space i.e., $\mu_0 = 4\pi \cdot 10^{-7}$ H/m and $\varepsilon_0 = 8.854212 \cdot 10^{-12}$ F/m. The measurement points and the source points are placed in the region surrounding the domain D . We consider four different incidence points and eight measurement points, i.e. $n_i = 4$ and $k_m = 8$; see Figure 4. To generate the incidence fields, we

Figure 4. Picture of the position of transmitters (Tx) and receivers (Rx) in the domain. Two generic scatterers are depicted in the domain D .

have used hard sources [32]. This means that we set a variation of the magnetic field directly where the transmitters are placed. Hence, we need to specify $f_n(t)$ in equation (1d) that in the TE_z case is $H_z = f(t)$, in the excitation points. As in [29], the excitation of the magnetic field was taken equal to the following

$$H_z(t) = \begin{cases} \frac{1}{\eta_0} \left(\frac{3}{10} \sin\left(\frac{2\pi t}{T_1}\right) + \sin\left(\frac{2\pi t}{T_2}\right) \right), & 0 \leq t \leq T_1, \\ 0 & T_1 < t, \end{cases}$$

for every n_i . Hence, we considered a truncated composition of sine wavefunctions with frequency of 20 kHz and 50 kHz, respectively.

To evaluate our inversion algorithm, we have considered an hidden dielectric square with side-length of ten cells and relative electrical permittivity $\epsilon_r = 3$. This square is placed such that the left lower corner has coordinate (25, 25) cell units in the computational domain. This square is depicted in Figure 5 with a eye-bird view. Hence, we solve the associated direct scattering problem and collect

Figure 5. Simulated scenario (left plot) and reconstructed scatterer after 20 iterations (right plot)

the predictions at the receivers for all time-steps in $(0, T)$. We also built synthetic measurements: we take the fields obtained using the scatterer domain which we would like to reconstruct and we added noise (thus avoiding inverse crimes). We denote the measurements corresponding to the n th incidence field and the k th receiver as E_{nk}^m and H_{nk}^m . We have used a white Gaussian noise such that the signal-to-noise ratio is $SNR = 10$ dB. For the two regularization terms we take $\beta = 10^{-10}$ and $\gamma = 10^{-10}$. This choice results from our experience.

To discuss the convergence properties of the algorithm, we introduce a measure of the reconstruction error as follows

$$\text{ER}_\varepsilon = \sqrt{\frac{\sum_{l=1}^L (\varepsilon^{(l)} - \tilde{\varepsilon}^{(l)})^2}{\sum_{l=1}^L (\varepsilon_0 - \tilde{\varepsilon}^{(l)})^2}},$$

where $L = 400$ is the number of cells of the scatterer domain D and the tilde indicates the true value of the property. Of course, the same formula is valid for the reconstruction of magnetic and conductive objects. In Figure 6 the decay of the reconstructed error along the iterations is depicted.

Figure 6. Reconstruction error along the iterations.

In the right plot of Figure 5, the reconstructed scatterer is presented. After 20 iterations, we obtain a good imaging of the true object. However, the reconstructed values are not constant in the square. In fact the edges tend to have greater values than those in the interior of the square. Instead of the true value $2.656 \cdot 10^{-11}$ F/m, we have as maximum value $2.695 \cdot 10^{-11}$ F/m and in the interior we have a minimum value of $2.161 \cdot 10^{-11}$ F/m. This means that we have a maximum $\varepsilon_r = 3.044$ and a minimum $\varepsilon_r = 2.440$. That is, the optimization algorithm is more accurate in correspondence of the edges.

4. A MODEL REDUCTION APPROACH: PROPER ORTHOGONAL DECOMPOSITION

In this section we utilize the POD method to derive a reduced-order model for the FDTD scheme. The performance of the reduced-order approach is studied for different frequencies.

4.1. The POD Galerkin scheme

First we describe the POD basis construction. Dealing with a TE_z wave, we have three field components, hence we build three basis set. First, we need to have the so-called *snapshots matrices*. To do so, we run an EM simulation using the FDTD method and we store the fields components in three matrices:

$$\begin{aligned} \mathbf{E}_x &= (\mathbf{E}_x^{1/2}, \dots, \mathbf{E}_x^{N_t+1/2}) \in \mathbb{R}^{M(N+1) \times (N_t+1)}, \\ \mathbf{E}_y &= (\mathbf{E}_y^{1/2}, \dots, \mathbf{E}_y^{N_t+1/2}) \in \mathbb{R}^{N(M+1) \times (N_t+1)}, \\ \mathbf{H}_z &= (\mathbf{H}_z^1, \dots, \mathbf{H}_z^{N_t+1}) \in \mathbb{R}^{MN \times (N_t+1)}. \end{aligned}$$

Because of the staggered grid, the three matrices have different number of rows. Let d_x denote the rank of $\mathbf{E}_x$. Then, $d_x \leq \min(M(N+1), N_t+1)$. Analogously, $d_y = \text{rank } \mathbf{E}_y \leq \min(N(M+1), N_t+1)$ and $d_z = \text{rank } \mathbf{H}_z \leq \min(NM, N_t+1)$.

Let us focus on the field component $\mathbf{E}_x$. The procedure is analogous for $\mathbf{E}_y$ and $\mathbf{H}_z$. In the POD approach, one would like to represent the columns $\mathbf{E}_x^j$, $1 \leq j \leq N_t+1$, of the matrix $\mathbf{E}_x$, the so-called *snapshots* by $\ell_x \leq d_x$ vectors $\psi_i \in \mathbb{R}^{M(N+1)}$, $i = 1, \dots, \ell_x$, in an optimal way. The basis

vectors ψ_i are given by the following optimization problem:

$$\begin{aligned} \min_{\psi_1, \dots, \psi_{\ell_x} \in \mathbb{R}^{d_x}} \quad & \sum_{j=1}^{N_t+1} \alpha_j \left\| \mathbf{E}_x^j - \sum_{i=1}^{\ell_x} \langle \mathbf{E}_x^j, \psi_i \rangle_{\mathbf{W}} \psi_i \right\|_{\mathbf{W}}^2 \\ \text{s.t.} \quad & \langle \psi_i, \psi_j \rangle_{\mathbf{W}} = \delta_{ij} \text{ for } i, j = 1, \dots, \ell_x, \end{aligned}$$

where $\langle \cdot, \cdot \rangle_{\mathbf{W}}$ denotes a weighted inner product with a symmetric, positive definite matrix $\mathbf{W} \in \mathbb{R}^{M(N+1) \times M(N+1)}$. We need to introduce this new inner product because the EM fields are functions, hence the L^2 inner product is the natural product that we need. Introducing an opportune $\mathbf{W}$ matrix, we can approximate numerically this product. Moreover, we introduced weights α_j , $j = 1, \dots, N_t + 1$ for the time dependency of the EM fields. More precisely, the α_j are the trapezoidal weights for the numerical integration over $[0, T]$.

The problem means that one would like to minimize the difference, for every snapshot $\mathbf{E}_x^j$, between the snapshot itself and its projection in the subspace defined by the basis vectors ψ_i , under the constraint of orthonormality property of the basis. Let us define $\mathbf{D} = \text{diag}(\alpha_1, \dots, \alpha_{N_t+1})$.

Using the Lagrangian framework and considering the ψ_i vectors as optimization variables, the optimality system is an $M(N+1) \times M(N+1)$ eigenvalue problem [15, 35]

$$\mathbf{Y}\mathbf{Y}^\top \psi_i = \lambda_i \psi_i, \quad i = 1, \dots, \ell_x,$$

with $\mathbf{Y} = \mathbf{W}^{1/2} \mathbf{E}_x \mathbf{D}^{1/2}$. We assume that the (real and nonnegative) eigenvalues are ordered as follows: $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{d_x} > \lambda_{d_x+1} = \dots = \lambda_{M(N+1)} = 0$.

Remark 4.1 1) According to the singular values decomposition properties we can solve the equivalent $(N_t + 1) \times (N_t + 1)$ eigenvalue problem:

$$\mathbf{Y}^\top \mathbf{Y} v_i = \lambda_i v_i, \quad i = 1, \dots, \ell_x,$$

Then, the ψ_i 's are given by

$$\psi_i = \frac{1}{\sqrt{\lambda_i}} \mathbf{Y} v_i, \quad i = 1, \dots, \ell_x.$$

2) If $\{\psi_i\}_{i=1}^{\ell_x}$ denotes the computed POD basis of rank ℓ_x , then we have the error formula

$$\sum_{j=1}^{N_t+1} \alpha_j \left\| \mathbf{E}_x^j - \sum_{i=1}^{\ell_x} \langle \mathbf{E}_x^j, \psi_i \rangle_{\mathbf{W}} \psi_i \right\|_{\mathbf{W}}^2 = \sum_{i=\ell_x+1}^{d_x} \lambda_i.$$

Thus, if the eigenvalues of $\mathbf{Y}\mathbf{Y}^\top$ decay rapidly, then $\sum_{i=\ell_x+1}^{d_x} \lambda_i$ is small. $\diamond$

Summarizing, for every field components we get a basis: $\Psi_x \in \mathbb{R}^{M(N+1) \times \ell_x}$, $\Psi_y \in \mathbb{R}^{N(M+1) \times \ell_y}$, $\Phi_z \in \mathbb{R}^{N M \times \ell_z}$ for the fields E_x , E_y , H_z , respectively.

The POD bases are used in the full discrete model (8) for a Galerkin ansatz:

$$\mathbf{E}_x^{m+1/2} \approx \Psi_x \mathbf{P}_x^{m+1/2}, \quad \mathbf{E}_y^{m+1/2} \approx \Psi_y \mathbf{P}_y^{m+1/2}, \quad \mathbf{H}_z^m \approx \Phi_z \mathbf{P}_z^m,$$

where $\mathbf{P}_x \in \mathbb{R}^{\ell_x}$, $\mathbf{P}_y \in \mathbb{R}^{\ell_y}$ and $\mathbf{P}_z \in \mathbb{R}^{\ell_z}$ have to be determined. We apply a Galerkin projection for the full discrete model. Instead of (8) we arrive at

$$\begin{pmatrix} \mathbf{M}_x^\ell & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_y^\ell \end{pmatrix} \begin{pmatrix} \mathbf{P}_x^{m+1/2} \\ \mathbf{P}_y^{m+1/2} \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{E_x}^\ell & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_{E_y}^\ell \end{pmatrix} \begin{pmatrix} \mathbf{P}_x^{m-1/2} \\ \mathbf{P}_y^{m-1/2} \end{pmatrix} + \begin{pmatrix} \mathbf{A}_y^\ell \mathbf{P}_z^m + \mathbf{W}_x^\ell \mathbf{J}_{sx}^m \\ \mathbf{A}_x^\ell \mathbf{P}_z^m + \mathbf{W}_y^\ell \mathbf{J}_{sy}^m \end{pmatrix} \quad (9a)$$

and set

$$\mathbf{P}_z^{m+1} = \mathbf{P}_z^m + \mathbf{B}_y^\ell \mathbf{P}_x^{m+1/2} - \mathbf{B}_x^\ell \mathbf{P}_y^{m+1/2}, \quad (9b)$$

where

$$\begin{aligned} \mathbf{M}_x^\ell &= \Psi_x^\top \mathbf{W} \mathbf{M}_x \Psi_x, & \mathbf{A}_{E_x}^\ell &= \Psi_x^\top \mathbf{W} \mathbf{A}_{E_x} \Psi_x, & \mathbf{A}_x^\ell &= \Psi_x^\top \mathbf{W} \mathbf{A}_x \Psi_x, \\ \mathbf{M}_y^\ell &= \Psi_y^\top \mathbf{W} \mathbf{M}_y \Psi_y, & \mathbf{A}_{E_y}^\ell &= \Psi_y^\top \mathbf{W} \mathbf{A}_{E_y} \Psi_y, & \mathbf{A}_y^\ell &= \Psi_y^\top \mathbf{W} \mathbf{A}_y \Psi_y, \\ \mathbf{B}_y^\ell &= \Psi_z^\top \mathbf{W} \mathbf{B}_y \Psi_x, & \mathbf{B}_x^\ell &= \Psi_z^\top \mathbf{W} \mathbf{B}_x \Psi_y, & \mathbf{W}_x^\ell &= \Psi_x^\top \mathbf{W}, & \mathbf{W}_y^\ell &= \Psi_y^\top \mathbf{W}, \end{aligned} \quad (10)$$

Notice that all matrices in (10) can be computed *off-line*, i.e., before we start the loop over $m = 1$ to N_t in (9). Moreover, we have used in (9b) that $\Psi_z^\top \mathbf{W} \Psi_z$ is the identity matrix.

To measure the error in the reduced-order model we introduce the quantity

$$\text{Err}_{E_x}(\ell) = \frac{\sum_{m=0}^{N_t} \alpha_m \|\mathbf{E}_x^{m+1/2} - \Psi_x \mathbf{P}_x^{m+1/2}\|_{\mathbf{W}}^2}{\sum_{m=0}^{N_t} \alpha_m \|\mathbf{E}_x^{m+1/2}\|_{\mathbf{W}}^2},$$

where α_m 's are the trapezoidal weights for the interval $[0, T]$. The quantities $\text{Err}_{E_y}(\ell)$ and $\text{Err}_{H_z}(\ell)$ are defined in an analogous way.

Remark 4.2

We mention that one can use a different ansatz for building POD basis as in, e.g. [4]. Hence, one compute the time average of the snapshots of a field component and subtract it from the corresponding snapshots matrix. We tested this approach too but its performance are similar to the approach presented in the section. $\diamond$

4.2. Numerical experiments

In this subsection we present numerical results from different test runs, where we study the performance of our POD Galerkin scheme. The amount of energy captured by an ℓ -rank basis is [15, 27, 35]

$$\mathcal{E}(\ell) = \sum_{i=1}^{\ell} \lambda_i \bigg/ \sum_{i=1}^d \lambda_i,$$

where the λ_i 's are the eigenvalues satisfying $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d > 0$. According to this, one can choose the percentage p of energy that the basis should keep and then calculate the minimum amount of vector basis required for that, using the formula

$$\ell = \text{argmin} \left\{ \mathcal{E}(\ell) : \mathcal{E}(\ell) \geq \frac{p}{100} \right\}.$$

We study now the behavior of the POD scheme using two different kind of source waveform and different frequencies. In the following, the medium used for getting the snapshots is the free space.

First, we consider the reduction of two different sinusoidal waves, with different frequencies. We choose for the first wave $f_1=5$ kHz and for the second one $f_2=20$ kHz. We consider these 2 simulations on the same space-time grid, so we define the grid parameter such that we have stability in the case of the highest frequency, f_2 .

Hence, using $p = 99.99\%$, the results are plotted in Table I. In both cases, we can compute the

field variable	sine $f_1 = 5$ kHz	sine $f_2 = 20$ kHz
E_x	$\ell_x = 6$	$\ell_x = 22$
E_y	$\ell_y = 6$	$\ell_y = 19$
H_z	$\ell_z = 9$	$\ell_z = 24$

Table I. Comparison of the number ℓ of POD basis needed in the case of sinusoidal waves with different frequencies ($p = 99.99\%$).

f eld variable	sine $f_1 = 5$ kHz	sine $f_2 = 20$ kHz
E_x	$\text{Err}_{E_x}(6) = 3 \cdot 10^{-3}$	$\text{Err}_{E_x}(22) = 9 \cdot 10^{-3}$
E_y	$\text{Err}_{E_y}(6) = 3 \cdot 10^{-3}$	$\text{Err}_{E_y}(19) = 4 \cdot 10^{-3}$
H_z	$\text{Err}_{H_z}(9) = 1 \cdot 10^{-2}$	$\text{Err}_{H_z}(24) = 1 \cdot 10^{-2}$

Table II. Comparison of the POD errors in the case of sinusoidal waves with different frequencies ($p = 99.99\%$) using the number of basis vectors in Table I.

POD-error in the reconstruction of the three f elds components, see Table II. We can conclude that for keeping the same amount of energy in the higher frequency case, we need more basis vectors than in the lower case. For every f eld component, in the case of f_2 , we need more than three times the basis number used in the f_1 case.

In the next simulation we considered two Gaussian pulses: the generic expression is stated in the following equation

$$s(t) = \exp\left(-\frac{(t - t_0)^2}{\tau^2}\right),$$

where $t_0 = 4.5\tau$ is the time shift used for avoiding starting the waveform in $t = 0$ with the maximum value of the pulse and τ determines the width of the pulse (for more details see [9]). In this case, we do not have a monochromatic source, i.e., we do not have a single frequency. Anyway, we can identify the maximum frequency of the pulse. Hence, we are interested in checking what happens if we choose different maximum frequencies. We use $f_{1max}=5$ kHz and $f_{2max}=10$ kHz and we used f_{2max} for having the right time step and space step in order to satisfy stability and sampling conditions. The number of POD basis functions are given in Table III. In Table IV we report on

f eld variable	Gauss $f_{1max} = 5$ kHz	Gauss $f_{2max} = 10$ kHz
E_x	$\ell_x = 2$	$\ell_x = 7$
E_y	$\ell_y = 2$	$\ell_y = 7$
H_z	$\ell_z = 3$	$\ell_z = 8$

Table III. Comparison of the number ℓ of POD basis needed in the case of Gaussian pulse waveforms with different maximum frequencies ($p = 99.99\%$)

the POD error for $p = 99.99\%$. As before, we see that if we have a higher maximum frequency, we

f eld variable	Gauss $f_{1max} = 5$ kHz	Gauss $f_{2max} = 10$ kHz
E_x	$\text{Err}_{E_x}(2) = 1 \cdot 10^{-3}$	$\text{Err}_{E_x}(7) = 1 \cdot 10^{-3}$
E_y	$\text{Err}_{E_y}(2) = 1 \cdot 10^{-3}$	$\text{Err}_{E_y}(7) = 2 \cdot 10^{-3}$
H_z	$\text{Err}_{H_z}(3) = 4 \cdot 10^{-3}$	$\text{Err}_{H_z}(8) = 1 \cdot 10^{-2}$

Table IV. Comparison of the POD errors in the case of Gaussian pulse waveforms with different maximum frequencies ($p = 99.99\%$) using the number of basis vectors in Table III.

need more basis functions in order to keep the same amount of energy as the lower frequency case. Moreover, the number of POD basis is related to the type of waveform used to having the snapshots. Even having the same frequencies (compare the cases f_1 for the sinusoidal case and f_{1max} for the Gaussian pulse), we need less basis functions in the Gaussian case. Hence, the number of basis functions is inf uenced by the kind of waveform and its frequency.

5. CONCLUSIONS

In this paper the problem of determining the EM properties ($\varepsilon(\mathbf{x}), \mu(\mathbf{x}), \sigma(\mathbf{x})$) of a hidden objects has be considered. This parameter identifcation problem is formulated in terms of a nonlinear

optimal control problem with Maxwell equations as side constraints. We have discussed the characterization of the solution to the optimization problem as the solution of an optimality system which involves Maxwell equations and adjoint Maxwell equations. Their solution provide the gradient of the reduced cost functional and we have used this gradient to define a successful iterative optimization technique to obtain a sequence of approximations of the EM properties. Then, in order to reduce the computational effort for the solution of the Maxwell equations, we have investigated consider a model reduction technique based on POD. The POD method for different kind of sources and frequencies and we concluded that this technique can catch the behavior of the snapshot with few basis functions.

In the future we would like to use the POD technique for having a basis set for solving the direct problem and another one for the adjoint one. Hence, we should consider the problem of updating the basis during the iterations of the optimization loop.

REFERENCES

1. Antoulas A. 2005 *Approximation of Large-Scale Dynamical Systems*. SIAM, Philadelphia.
2. Bennett C. 1981. *Time domain inverse scattering*. IEEE Transactions on antennas and propagation, 29:213-219.
3. Berenger J. 1994. *A perfectly matched layer for the absorption of electromagnetic waves*. Journal of Computational Physics, 114:185-200.
4. Chatterjee A. 2000. *An introduction to the proper orthogonal decomposition*. Current Science, 78:808-817.
5. Chen Y, Hesthaven J, Maday Y. 2011. *A seamless reduced basis element method for 2D Maxwell's problem: an introduction*. Spectral and High Order Methods for Partial Differential Equations-Selected papers from the ICASOHOM'09 conference, 76:141-152.
6. Chen Y, Hesthaven J, Maday Y, Rodriguez J, Zhu X. 2011. *Certified reduced basis method for electromagnetic scattering and radar cross section estimation*. Submitted.
7. Delbary F, Erhard K, Kress R, Potthast R, Schulz J. 2008. *Inverse electromagnetic scattering in a two-layered medium with an application to mine detection*. Inverse Problems, 24:1-25.
8. Du J, Zhu J, Luo Z, Navon I.M. 2009. *An optimizing finite difference scheme based on proper orthogonal decomposition for CVD equations*. Communications in Numerical Methods in Engineering, 27:78-94.
9. Elsherbeni A, Demis D. 2009. *The Finite-Difference Time-Domain Method for Electromagnetics with Matlab Simulations*. Scitech Publishing. Inc., Raleigh.
10. Fares B, Hesthaven J.S., Maday Y, Stamm B. 2011. *The reduced basis method for the electric field integral equation*. Submitted.
11. Franceschetti G. 1998. *Campi elettromagnetici*. Bollati Boringhieri, Torino.
12. Ganesh M, Hesthaven J, Stamm B. 2011 *A reduced basis method for multiple electromagnetic scattering in three dimensions*. Preprint submitted to Journal of Computational Physics.
13. Hinze M, Pinnau R, Ulbrich M, Ulbrich S. 2009. *Optimization with PDE Constraints*. Springer-Verlag, Berlin.
14. Hinze M, Volkwein S. 2005. *Proper orthogonal decomposition surrogate models for nonlinear dynamical systems: error estimates and suboptimal control*. In Reduction of Large-Scale Systems, P. Benner, V. Mehrmann, D.C. Sorensen (eds.), Lecture Notes in Computational Engineering, 45:261-306.
15. Holmes P, Lumley J.L., G. Berkooz G. 1996 *Turbulence, Coherent Structures, Dynamical Systems and Symmetry*. Cambridge Monographs on Mechanics, Cambridge University Press.
16. Ito K, K. Kunisch. 2008. *Lagrange Multiplier Approach to Variational Problems and Applications*. SIAM, Philadelphia.
17. Jin J. 2010. *Theory and Computation of Electromagnetic Fields*. Wiley, Hoboken.
18. Kang N, Chung Y, Cheon C, Jung H. 2002. *A new 2-D image reconstruction algorithm based on FDTD and design sensitivity analysis*. IEEE Transactions on Microwave Theory and Techniques, 50:2734-2740.
19. Kress R. 2009. *Inverse scattering theory*. Notes Study, Göttingen.
20. Leis R. 1988. *Initial Boundary Value Problems in Mathematical Physics*. John Wiley, New York.
21. Mancini R. 2009. *An Adjoint-Based Optimization Scheme for Solving Time-Domain Electromagnetic Inverse Scattering Problems*. Master thesis, Benevento, Italy.
22. Maurer H, Zowe J. 1979. *First and second-order necessary and sufficient optimality conditions for infinite-dimensional programming problems*. Math. Programming, 16:98-110.
23. Monk P, Süli E. 1994. *A convergence analysis of Yee's scheme on nonuniform grids*. SIAM J. Numer. Anal., 31:393-412.
24. Mur G. 1981. *Absorbing boundary conditions for the finite-difference approximation of the time-domain electromagnetic-field equations*. IEEE Transactions On Electromagnetic Compatibility, 23 (4): 377382.
25. Noack B.R., Morzyński M, Tadmor G. 2011. *Reduced-Order Modelling for Flow Control*. CISM Courses and Lectures, vol. 528, Springer-Verlag, Wien.
26. Nocedal J, Wright S. 2000. *Numerical Optimization*. Springer, New York.
27. Pinnau R. 2008. *Model reduction via proper orthogonal decomposition*. Model Order Reduction: Theory Research Aspects and Applications, Springer Series Mathematics in Industry, Vol. 13.
28. Pozar D. 2005. *Microwave Engineering*. Wiley, Hoboken.
29. Rekanos I. 2003. *Time-domain inverse scattering using Lagrange multipliers: an iterative FDTD-based optimization technique*. J. of Electromagn. Waves and Appl., 17:271-289.

30. Semnani A, Kamyab M. 2007. *An enhanced method for inverse scattering problems using fourier series expansion in conjunction with FDTD and PSO*. Progress In Electromagnetics Research, 76:45-64.
31. Sun P, Luo Z, Zhou Y. 2010. *Some reduced finite difference schemes based on a proper orthogonal decomposition technique for parabolic equations*. Applied Numerical Mathematics, 60:154-164.
32. Taflov A, Hagness S. 2000. *Computational Electrodynamics: The Finite-Difference Time-Domain Method*. Artech House, Norwood.
33. Tanaka T, Takenaka T, He S. 1999. *An FDTD approach to the time-domain inverse scattering problem for an inhomogeneous cylindrical object*. Microwave And Optical Technology Letters, 20:72-77.
34. Tröltzsch F. 2010. *Optimal Control of Partial Differential Equations. Theory, Methods and Applications*. American Mathematical Society, Providence.
35. Volkwein S. 2011. *Model Reduction using Proper Orthogonal Decomposition*. Lecture Notes, University of Konstanz.
www.math.uni-konstanz.de/numerik/personen/volkwein/teaching/POD-Vorlesung.pdf
36. Yee K. 1966. *Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media*. IEEE Trans. Antennas and Propagation, AP-16:302-307.